

# Anomalous Heat Conduction in Carbon Nanowire

Gang Wu and Jinming Dong

National Laboratory of Solid State Microstructures, Department of Physics, Nanjing University, Nanjing, 210093, People's Republic of China

## Abstract

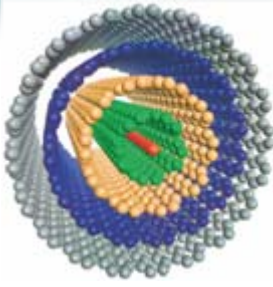
Heat conduction of a real quasi-one dimensional materials, Heat conduction of a real quasi-one dimensional materials, the finite length carbon nanowires (CNWs), inserted into the single-walled carbon nanotube (SWNT) has been studied by the molecular dynamical method, in which both of the longitudinal as well as transverse motions of the chain atoms in the SWNT have been permitted. It is found that the thermal conductivity  $\kappa$  of the carbon nanowire is very high at room temperature, and diverges more likely with the chain length logarithmically.

## Models and Method

### System in practice:

X. Zhao *et al.*, Phys. Rev. Lett. 90, 187401 (2003)

The innermost tube is the armchair (5,5) with a radius of  $\sim 3.5 \text{ \AA}$



### Our model: CNW@ (5, 5) SWNT

The interaction between chain atoms is simulated by the Tersoff-Brenner bond order potential, and the interaction between carbon chain and outside nanotube is described by Lennard-Jones(LJ) potential,

$$u(x) = 4\epsilon \left[ -\left(\frac{\sigma}{x}\right)^6 + \left(\frac{\sigma}{x}\right)^{12} \right].$$

The carbon atoms on outside nanotube is assumed to be distributed continuously, which is well known as the continuum model.

The average equilibrium distance between the chain atoms is set to be  $a = 1.84 \text{ \AA}$ , which means there are four carbon atoms in three periods of outside armchair nanotube.

Two atoms at each end of the CNW are subject to heat baths at  $T_L$  and  $T_R$  respectively, which usually can be simulated by Nosé-Hoover thermostats.

$$\ddot{\vec{r}} = -\zeta \dot{\vec{r}} + \vec{f},$$

$$\dot{\zeta} = \frac{1}{Q} \left( \sum_i \frac{\vec{p}_i^2}{m_i} - g k_B T \right), \quad Q = g k_B T \tau^2.$$

Fixed boundary conditions are assumed for extra two atoms at each end of the CNW.

$T_L$  and  $T_R$  are kept as 0.03 and 0.025, which correspond to real 290K and 348K in practice, respectively.

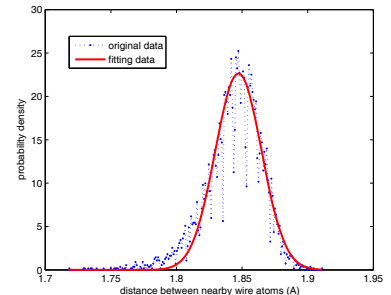
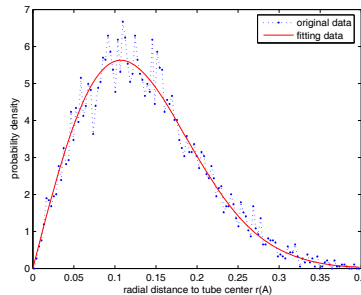
The time step is chosen from  $h = 0.01$  to  $0.05$  in the unit of  $0.035267 \text{ ps}$ . Typical total MD steps are taken as  $10^7$  to  $10^8$ .

Eighth-order Runger-Kutta algorithm is employed to solve the ordinary differential equations.

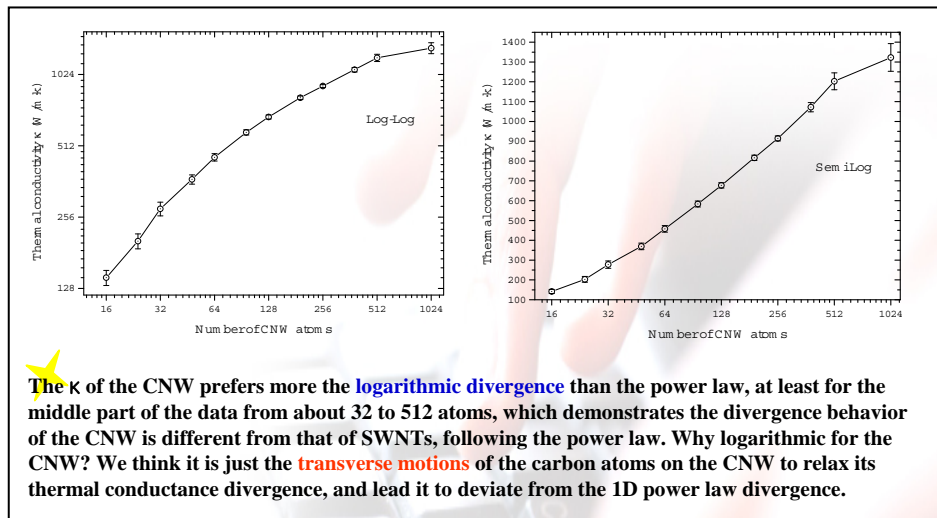
Comparison between the thermal conductivities of both 1D carbon chain and the quasi-1D CNW clearly show that it is indeed the transverse motions of the carbon atoms on the CNW to cause its logarithmic thermal conductance divergence.

## Numerical Results and Discussions

### The distribution of CNWs atoms position under model condition



At about room temperature, the distances among the CNW atoms in the stable state are almost equal, and the deviation displacement from the equilibrium position obeys the Gauss distribution. The radial distribution of the CNW atoms obeys the Weber distributions ( $n=2$ ).

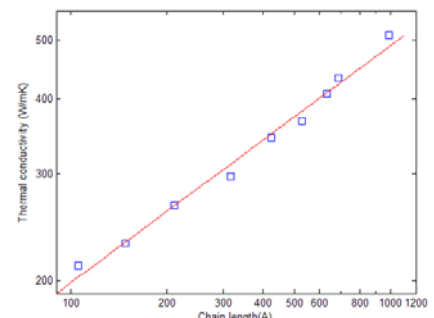


The  $\kappa$  of the CNW prefers more the logarithmic divergence than the power law, at least for the middle part of the data from about 32 to 512 atoms, which demonstrates the divergence behavior of the CNW is different from that of SWNTs, following the power law. Why logarithmic for the CNW? We think it is just the transverse motions of the carbon atoms on the CNW to relax its thermal conductance divergence, and lead it to deviate from the 1D power law divergence.

### The influence of the transverse motions:

The thermal conductivity of perfect 1D carbon chains connected by the Tersoff-Brenner bond order potential, in which, transverse motions are not permitted. The initial equilibrium distance between neighboring atoms are set to be  $1.65 \text{ \AA}$ .

The  $\kappa$  diverges with chain length as,  $\kappa \propto L^\beta$ , with  $\beta \approx 0.39 \pm 0.02$ .



The heat conduction of a carbon chain inserted into a (5, 5) SWNT has been studied by nonequilibrium molecular dynamics method, in which both longitudinal and transverse motions of the chain atoms are permitted. The influence of outside nanotube has been simulated by a continuum model. It is found that heat conduction  $\kappa$  of CNW does not obey the Fourier law, and diverges with CNW length  $L$  as  $L^{0.39 \pm 0.02}$ .

